In-Medium Similarity Renormalization Group for Open-Shell Nuclei

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We present a nonperturbative derivation of effective valence-shell Hamiltonians in the framework of the recently developed in-medium similarity renormalization group (IM-SRG). As a first application, we calculate the spectra of *p*- and *sd*-shell nuclei, ^{6}Li and ^{18}O, based on evolved chiral nucleon-nucleon interactions. For ^{6}Li, the spectrum is in very good agreement with ab-initio results. For ^{18}O, the IM-SRG provides a new method for the shell model to systematically go beyond effective interaction techniques based on diagrammatic expansions.

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Introduction.– Advances in ab-initio methods for nuclear structure combined with nuclear forces based on chiral effective field theory (EFT) have lead to many exciting developments for light nuclei and medium-mass nuclei around closed-shell configurations (see, e.g., Refs. [1]). For open-shell systems with many valence nucleons, however, the shell model remains the most successful approach to understand and predict nuclear structure, including the evolution of shell structure with changing neutron and proton numbers, properties of ground and excited states, and electroweak transitions [2]. Moreover, the shell model has recently revealed new insights to the impact of long-range tensor [3] and three-nucleon forces [4] in neutron-rich nuclei. These are dominated by pion exchanges, which provides a link between nuclear structure and developments in chiral EFT interactions. Despite the many successes of the shell model, the microscopic derivation of effective interactions and operators among valence nucleons from nuclear forces is still largely based on perturbative approaches where the convergence remains an open problem.

In this Letter, we present a new nonperturbative derivation of effective valence-shell Hamiltonians in the framework of the in-medium similarity renormalization group (IM-SRG), which we recently developed for closed-shell nuclei [5, 6]. The IM-SRG is based on a renormalization group evolution that decouples degrees of freedom that are not relevant for the problem of interest. We show how the IM-SRG can be generalized to open-shell systems away from doubly-magic nuclei. For ^{6}Li, we present first results for the ground-state energy and spectrum in very good agreement with ab-initio methods. We then discuss for ^{18}O how the IM-SRG goes significantly beyond effective interaction techniques based on diagrammatic expansions [7], opening up a promising new method to connect nuclear forces and the shell model.

IM-SRG and generator choices.– The IM-SRG starts from a Hamiltonian H that is normal ordered with respect to a finite-density reference state $|\Phi\rangle$ (e.g., the Hartree-Fock ground state):

$$H = E_0 + \sum_{ij} f_{ij} \{a_i^\dagger a_j\} + \frac{1}{2!^2} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j^\dagger a_l a_k\} , \quad (1)$$

where the normal-ordered strings of creation and annihilation operators obey $\langle\Phi|\{a_i^\dagger \cdots a_j\}|\Phi\rangle = 0$. We include normal-ordered 0-, 1-, and 2-body operators, E_0, f, and Γ, which approximately include induced 3- and higher-body interactions, and solve the IM-SRG flow equations to obtain the evolved Hamiltonian $H(s)$ [5]. We refer to this truncation as IM-SRG(2) since we keep up to normal-ordered 2-body operators. The evolution is equivalent to a series of unitary transformations that are designed to evolve $H(s)$ as $s \to \infty$ to an appropriately defined "diagonal" part $H^{\rm d}(s)$ [8, 9]:

$$H(s) = U(s) H U^\dagger(s) \equiv H^{\rm d}(s) + H^{\rm od}(s) \to H^{\rm d}(\infty) . \quad (2)$$

The unitary transformation $U(s)$ is determined by the generator $\eta(s) \equiv [dU(s)/ds]\, U^\dagger(s)$, which is constructed from the diagonal part,

$$\eta(s) = [H^{\rm d}(s), H(s)] = [H^{\rm d}(s), H^{\rm od}(s)] , \quad (3)$$

and guarantees that the "off-diagonal" coupling $H^{\rm od}$ is driven to zero with increasing s.

For the ground state of closed-shell nuclei, one eliminates all terms that couple the reference state $|\Phi_c\rangle$ to the rest of the Hilbert space. This is achieved when the matrix elements between $|\Phi_c\rangle$ and all n-particle–n-hole states vanish, $\langle npnh|\, H(\infty)\, |\Phi_c\rangle = 0$. Therefore, one takes $H_c^{\rm od}$ to be composed of all 1- and 2-body operators that connect hole (h) with particle (p) states so that $\{H_c^{\rm od}\} = \{f_{ph}, \Gamma_{pp'hh'}\}$ plus hermitian conjugates, as was demonstrated in Ref. [5].

For open-shell nuclei, particle states p can either be valence particles or particle states above the valence space,

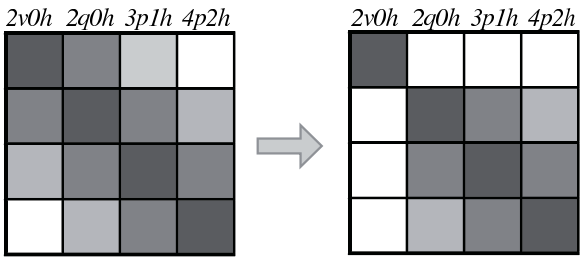

FIG. 1: Schematic illustration for the valence-space decoupling by the IM-SRG evolution from $H(s=0) \to H(\infty)$ for two valence nucleons.

which we denote by v and q respectively. We want to decouple states that are not in the valence space, spanned by $|\Phi_v\rangle = \{a^\dagger_{v_1} \cdots a^\dagger_{v_N}\}|\Phi_c\rangle$, where N is the number of valence nucleons and $|\Phi_c\rangle$ is the reference state for the core nucleus with A_c nucleons. This can be realized by defining $H^{\rm od}$ through the set of matrix elements

$$\{H_1^{\rm od}\} = \{f_{ph}, f_{qv}, \Gamma_{pp'hh'}, \Gamma_{pp'(vh\,{\rm or}\,hv)}, \Gamma_{(pq\,{\rm or}\,qp)vv'}\}\,, \tag{4}$$

where $p = v, q$, plus hermitian conjugates. As an alternative generator choice $H_2^{\rm od}$, we also drive the one-body part to diagonal, so that we define

$$\{H_2^{\rm od}\} = \{H_1^{\rm od}, f_{pp'}, f_{hh'}\}\,. \tag{5}$$

These generators both lead to a diagonal part $H^{\rm d}_{1,2}$ where states outside the valence space are decoupled by the IM-SRG flow, illustrated in Fig. 1, leading to

$$PH^{\rm d}_{1,2}(\infty)Q = QH^{\rm d}_{1,2}(\infty)P = 0\,, \tag{6}$$

with $P = \sum_v |\Phi_v\rangle\langle\Phi_v|$ and $Q = 1 - P$. The off-diagonal parts in Eqs. (4) and (5) can also be derived using the counting operator $C = \sum_i c_i\{a_i^\dagger a_i\}$, with $c_i = 1, 0, -1$ for q, v, h states, respectively. The C operator counts the number of excitations on top of a valence-space state $|\Phi_v\rangle$. It is then straightforward to verify that the above choices of $H^{\rm od}_{1,2}$ ensure $0 = CH(\infty)|\Phi_v\rangle = [C, H(\infty)]|\Phi_v\rangle$, which leads to the decoupling of valence-space states from arbitrary excitations.

After the IM-SRG(2) evolution, the effective valence-shell Hamiltonian is given by $H_{\rm eff} \equiv PH^{\rm d}_{1,2}(\infty)P - E_0^{A_c}$, where $E_0^{A_c}$ is the 0-body piece of the evolved Hamiltonian corresponding to the ground-state energy of the core. We then solve a reduced eigenvalue problem in the N valence-particle space,

$$H_{\rm eff}\,|\chi_n\rangle = (E_n^A - E_0^{A_c})\,|\chi_n\rangle\ . \tag{7}$$

Results.– We next present first applications of the IM-SRG to two open-shell nuclei, ^{6}Li and ^{18}O, consisting of two valence nucleons on top of the closed-shell nuclei ^{4}He and ^{16}O. All results are based on the SRG-evolved

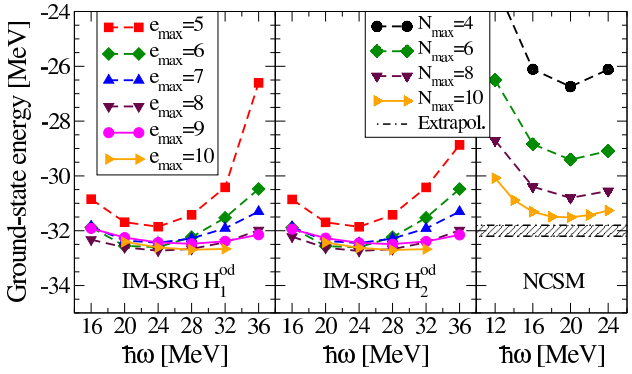

FIG. 2: The ground-state energy of ^{6}Li versus harmonic-oscillator parameter $\hbar\omega$ obtained by a diagonalization of the IM-SRG(2) $H_{\rm eff}$ in the p-shell, using generators $H_1^{\rm od}$ and $H_2^{\rm od}$ (left and center panels). The flow equations are solved in the HF basis truncated to $e_{\rm max} = \max(2n + l)$ single-particle excitations. For comparison we show in the right panel the convergence with increasing $N_{\rm max}$ of the NCSM energy [12], where the dot-dashed band is the extrapolated result.

($\lambda = 2.0\,{\rm fm}^{-1}$) N^{3}LO NN potential of Ref. [10]. We begin with ^{6}Li, which is a sufficiently light nucleus to allow a direct comparison of our IM-SRG(2) results with exact diagonalizations of the 6-body problem using the No-Core Shell Model (NCSM). For the IM-SRG calculations, the flow equations are solved in the Hartree-Fock (HF) basis of the initial Hamiltonian truncated to $e_{\rm max} = \max(2n + l)$ single-particle excitations. The resulting $H_{\rm eff}$ is then diagonalized in the p-shell to obtain the ^{6}Li energy levels with respect to the ground-state energy of the ^{4}He core. There is a subtlety that arises due to the self-bound nature of atomic nuclei. As we wish to minimize spurious center-of-mass motion, we work with the intrinsic Hamiltonian $H_{\rm int} = H - \mathbf{P}^2/(2mA)$ where $\mathbf{P} = \sum_i \mathbf{p}_i$ and $A = 6$ for ^{6}Li. Therefore, the eigenvalues of $H_{\rm eff}$ correspond to the excitation energies of ^{6}Li with respect to the ground state of the unphysical ^{4}He nucleus obtained using $H_{\rm int}$ with $A = 6$. Consequently, to get the absolute ground-state energy of ^{6}Li, we do a separate IM-SRG(2) calculation of the ground state of the unphysical ^{4}He core and add this to the eigenvalues of $H_{\rm eff}$. We have checked that for large $e_{\rm max}$ spaces, the center-of-mass factorizes as in Ref. [11].

Figure 2 shows the convergence of the ground-state energy of ^{6}Li with increasing $e_{\rm max}$ excitations. The left panels give the IM-SRG(2) results using the two different generators $H_1^{\rm od}$ and $H_2^{\rm od}$, while the right panel shows NCSM energies [12] for comparison. Since the single-particle $e_{\rm max}$ truncation is different than the NCSM

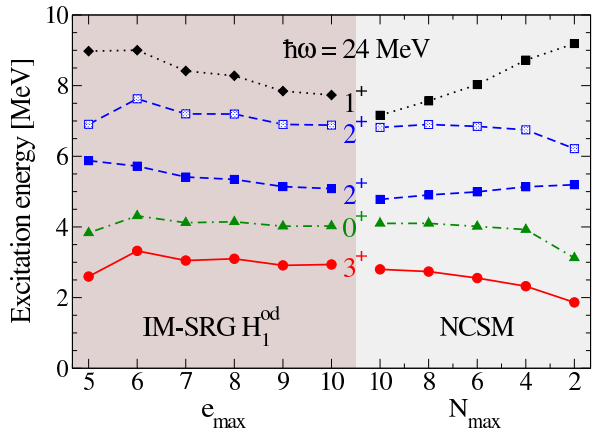

FIG. 3: Convergence as a function of $e_{\max}$ of the excitation energies of ^{6}Li obtained by diagonalizing the IM-SRG(2) $H_{\rm eff}$ in the p-shell using the $H_1^{\rm od}$ generator. The HF basis at a fixed $\hbar\omega = 24\,$MeV is used for the IM-SRG(2) calculations. For comparison we show the convergence with $N_{\max}$ of the NCSM energies at the same $\hbar\omega$ value [12].

$N_{\max}$, the convergence pattern of the two methods is expected to be different (an $e_{\max}$ space for the same value is substantially larger). The IM-SRG(2) ground-state energy converges to $-32.7(3)\,$MeV, where contributions from normal-ordered three-body interactions are expected to be repulsive (similar to triples correction in coupled-cluster calculations) [5], in very good agreement with the extrapolated NCSM value $-32.0(2)\,$MeV [12]. The generator dependence in Fig. 2 is found to be very weak, indicating that the error from truncating the IM-SRG equations to two-body operators is indeed small.

Next, we study the convergence properties of the low-lying excited states of ^{6}Li. The left panel of Fig. 3 shows the convergence of the IM-SRG(2) spectrum as a function of $e_{\max}$ at a fixed value of $\hbar\omega = 24\,$MeV. However, the $\hbar\omega$ dependence is very weak in the HF basis for large $e_{\max}$. The right panel shows the convergence of the NCSM spectrum with $N_{\max}$. The low-lying 3^+, 0^+ and two 2^+ states converge rather well and are in reasonable agreement with the NCSM results. The high-lying 1^+ state is not yet converged even at the largest space for both methods. As the convergence is very poor in the NCSM with a harmonic-oscillator basis, this could indicate that this state has an extended structure.

Our results for ^{6}Li are very encouraging and show that the IM-SRG provides a new method to derive effective valence-shell Hamiltonians that accurately reproduce the low-lying spectrum obtained with ab initio methods, but at a polynomial scaling $\sim N_h^4 N_p^2$ with the number of hole and particle orbits. Recently, other methods have been explored for open-shell nuclei, including two-particle attached coupled-cluster theory [13], which however leads to nonhermitian effective Hamiltonians, and the NCSM with a core [14], which requires a NCSM solution of the full problem and is therefore limited to lighter nuclei.

Turning to ^{18}O, where an exact diagonalization of the 18-body problem is out of reach, we compare our IM-SRG(2) results for the spectrum in Fig. 4 to calculations based on diagrammatic expansions (called the Q-box expansion) commonly used to derive effective shell-model Hamiltonians [7]. In this context, one can also understand our choices for $H_{1,2}^{\rm od}$ as follows. When one derives effective interactions among valence nucleons using perturbation theory, then the many-body diagrams contain at least one vertex of $\Gamma_{pp'hh'}$, $\Gamma_{pp'(vh\,\text{or}\,hv)}$, or $\Gamma_{(pq\,\text{or}\,qp)vv'}$. These interaction vertices are precisely the off-diagonal part driven to zero under the IM-SRG evolution. Therefore, the effective interactions among valence nucleons are directly given by $PH_{1,2}^{\rm d}(\infty)P$ (only at finite s, there would be perturbative corrections). For a clear comparison to shell-model calculations for ^{18}O, we use the same empirical single-particle energies for the one-body part of $H_{\rm eff}$ in both IM-SRG and Q-box calculations, that is we replace the calculated one-body part in the IM-SRG by the empirical USDb [16] single-particle energies.

The left panel of Fig. 4 compares the low-lying ^{18}O excitation energies obtained by diagonalizing the sd-shell $H_{\rm eff}$ derived from the IM-SRG(2) and the Q-box expansion. We also give the experimental energies [15], although good agreement with experiment is not required since three-nucleon (3N) forces are not included in the initial Hamiltonian and we do not fine-tune the single-particle basis to reproduce the experimental root-mean-square radius (see below). All calculations are performed in the HF basis. For the perturbative Q-box results, the open symbols correspond to an $H_{\rm eff}$ that is calculated at first, second, and third-order, while the solid symbols include higher-order folded-diagram contributions to remove the energy dependence of induced interaction vertices [7]. For the IM-SRG(2) results, as for ^{6}Li, we observe negligible differences in the calculated spectra for the two generators $H_1^{\rm od}$ and $H_2^{\rm od}$. This implies that the truncation of the flow equations to two-body operators is a very good approximation. The IM-SRG(2) energies are similar to the results based on the perturbative Q-box expansion, where some differences from the "best" results ($Q^{(3)}$ plus folded-diagram contributions) are expected because the IM-SRG is a nonperturbative method that includes many higher-order terms.

The poor agreement with experiment in Fig. 4 compared to conventional shell-model calculations might be surprising. The reason for this discrepancy is that conventional calculations include additional phenomenology that improves agreement with experiment, but weakens the connection with the underlying Hamiltonian and microscopic many-body theory. This can be understood from the right panel of Fig. 4, which displays the $\hbar\omega$ dependence of the ^{18}O excitation energies for second-order

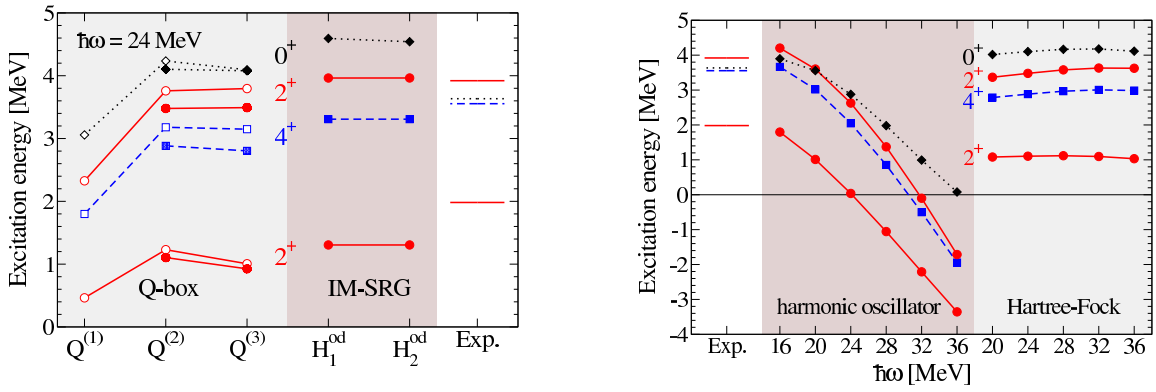

FIG. 4: Left panel: Excitation energies of ^{18}O obtained by diagonalizing the IM-SRG(2) $H_{\rm eff}$ in the *sd*-shell, compared with results obtained at first ($Q^{(1)}$), second ($Q^{(2)}$) and third ($Q^{(3)}$) order in the Q-box expansion [7] for effective valence-shell interactions (the filled symbols include higher-order folded-diagram contributions). All results are for $\hbar\omega = 24\,$MeV, but a HF basis is used. For comparison, we also show the experimental energies [15]. Right panel: Excitation energies of ^{18}O versus $\hbar\omega$ calculated at the second-order Q-box level (plus folding) in a harmonic-oscillator and HF basis. For the results of both panels, an $e_{\rm max} = 8$ space was used, and to simplify the comparison, the calculations used single-particle energies from the USDb interaction [16] for the diagonalization in the *sd*-shell.

Q-box calculations performed in the harmonic-oscillator (HO) and the HF basis. The HO-based spectrum exhibits a very strong $\hbar\omega$ dependence, while calculations in the HF basis are nearly independent of $\hbar\omega$. Conventional calculations of $H_{\rm eff}$ work in the HO basis with $\hbar\omega \approx 45A^{-1/3} - 25A^{-2/3}$ chosen to give the same root-mean-square radius as a sphere of uniform density. The fine-tuning of $\hbar\omega$ can therefore be understood as a phenomenological means to build in the correct saturation properties of nuclei, which are known to be deficient in ab-initio calculations starting from Hamiltonians without three-nucleon forces [9]. Our IM-SRG calculations present a microscopically-derived $H_{\rm eff}$, but the incorrect saturation properties of the initial NN-only Hamiltonian translate into a poor description of the ^{18}O spectrum compared to empirical calculations carried out in a HO basis (at $\hbar\omega \approx 14\,$MeV for ^{18}O).

Conclusions.– We have shown that the IM-SRG can be successfully generalized to open-shell systems and to a nonperturbative derivation of effective valence-shell Hamiltonians. The IM-SRG evolution decouples the physics of valence nucleons from the full Hilbert space, enabling exact diagonalizations in the valence space that are impossible in the full problem where all nucleons are active. First results were presented for ^{6}Li, with ground-state and excited-state energies in very good agreement with ab-initio methods. We then applied the IM-SRG to ^{18}O and compared our results to those obtained from conventional perturbative calculations of $H_{\rm eff}$, demonstrating that the IM-SRG provides a first viable nonperturbative approach to derive effective interactions for the shell model from nuclear forces. Work is in progress to extend the IM-SRG to extended valence spaces, to effective operators and to the inclusion of three-nucleon forces.

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